ABSTRACT

Modular Computational Models for Predicting the Pharmaceutical Properties of Chemical Compounds

The methods of the invention allow for the construction and/or use of modular computational models to accurately predict the therapeutic properties, including both therapeutic potency and one or more ADMET properties, of all or part of a chemical compound. The modular computational models can be used to rapidly screen libraries of chemical compounds, and reliably identify small subsets of those chemical compounds that have desirable therapeutic potency and ADMET properties, and are thus the best overall drug candidates.